# Romit Maulik

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## Research interests

Scientific machine learning, high-performance computing, computational fluid dynamics, reduced-order modeling, numerical methods, stochastic processes, geophysical forecasting.

## Education

PhD. Mechanical & Aerospace Engineering, Oklahoma State University. **2016-2019**

M.S. Mechanical & Aerospace Engineering, Oklahoma State University. **2013-2015**

B.E. Mechanical Engineering, Birla Institute of Technology, India. **2008-2012**

## Positions held

**Starting July 2023**
Assistant Professor, Information Sciences and Technology, Institute of Computational and Data Sciences, Pennsylvania State University
&
Joint Appointment, Mathematics and Computer Science Division, Argonne National Laboratory.

**Jun, 2021 - Present**
Assistant Computational Scientist, Mathematics and Computer Science, Argonne National Laboratory.

**Oct, 2020 - Present**
Research Assistant Professor, Department of Applied Mathematics, IIT-Chicago.

**Jun, 2019 - May, 2021**
Margaret Butler Postdoctoral Fellow, Leadership Computing Facility, Argonne National Laboratory.

**Jan, 2019 - May, 2019**
Predoctoral Appointee - Mathematics and Computer Science Division, Argonne National Laboratory.

**Jan, 2016 - Jan, 2019**
Research Assistant - Computational Fluid Dynamics Laboratory, Oklahoma State University.

**Aug, 2013 - Jul, 2015**
Research Assistant - Computational Biomechanics Laboratory, Oklahoma State University.

**Jan, 2013 - Dec, 2018**
Teaching Assistant (Introductory Dynamics, Introductory Fluid Mechanics, Practical CFD) - Mechanical & Aerospace Engineering, Oklahoma State University.

**Aug, 2012 - Aug, 2013**
Design Engineer - Tata Technologies Limited, India.

# Honors & awards

Invited participant, SIAM Convening on Climate Science, Sustainability, and Clean Energy (DMS 2227218), Tysons Corner, Virginia, October 10-12, 2022. White paper available here: `https://sinews.siam.org/Details-Page/change-the-conversation-at-the-local-level`.

Best paper award with Sudeepta Mondal, Gina M. Magnotti, Bethany Lusch, and Roberto Torelli. ASME Internal Combustion Engine Fall Conference, 2021.

Impact Argonne Award, September, 2021: 'For tackling several climate model challenges and advancing the field of downscaled climate modeling and impact analysis'.

Margaret Butler Fellow, Argonne Leadership Computing Facility, Argonne National Laboratory, 2019-2021.

SIAM Travel Grant: 2019 SIAM Conference on Computational Science and Engineering, Spokane, WA, 2019.

Outstanding Graduate Student, College of Engineering Architecture and Technology, Oklahoma State University, 2018.

Graduate College Robberson Summer Research Fellowship, Oklahoma State University, 2018.

SIAM TX-LA Section Travel Grant, Texas Applied Mathematics and Engineering Symposium, 2017.

Graduate Student Travel Grant, American Physical Society - Division of Fluid Dynamics, 2017.

Graduate Student Travel Grant, Graduate Program Student Government Authority, Oklahoma State University, 2017.

FGSA Travel Grant for Excellence in Graduate Research, American Physical Society, 2017.

John Brammer Fellowship, Oklahoma State University, 2016.

Graduate College Top Tier Fellowship, Oklahoma State University, 2016.

# Funding & support

(Active) Community Research on Climate and Urban Science, U.S. Department of Energy (Biological and Environmental Research), Role: Co-PI (PI-Cristina Negri); Year 2022-2027. Amount: $25000000.

(Active) Inertial neural surrogates for stable dynamical prediction, U.S. Department of Energy (Advanced Scientific Computing Research), Role: PI; Year 2021-2024. Amount: $3457000.

(Active) AI emulator assisted data assimilation, Future computing, LDRD-Prime, Argonne National Laboratory, U.S. Department of Energy. Role: Co-PI (PI-Rao Kotamarthi); Year: 2021–2023. Amount: $1240000.

(Active) RAPIDS2: A SciDAC Institute for Computer Science, Data, and Artificial Intelligence, U.S. Department of Energy. Role: Senior Personnel (PI-Rob Ross); Year: 2020–2025. Amount: $4236400.

(Active) Prediction-to-Mitigation with Digital Twins of the Earth's Weather, MOE Tier-2 Grant, Singapore. Role: External Collaborator (PI-Gianmarco Mengaldo); Amount: S$685000.

(Finished) A Scalable, Energy Efficient HPC Environment for AI-Enabled Science, National Science Foundation Collaborative PPoSS funding. Role: Co-PI (PI-Zhiling Lan); Year 2021-2022. Amount: $150,000.

(Finished) SambaWF: Highly resolved surrogate models for weather forecasting, LDRD-Expedition, Argonne National Laboratory, U.S. Department of Energy. Role: PI; Year: 2021-2021. Amount: $50,000.

(Finished) Scalable machine learning for turbulence closure and reduced-order modeling, Margaret Butler Fellowship, Role: PI, Year: 2019-2021. Amount: $400,000 (approximately).

# Supervising

Shivam Barwey, PhD, Postdoctoral Fellow, Argonne Leadership Computing Facility, Argonne National Laboratory (2022-Present).

Jonah Botvinick Greenhouse (Cornell University): Deep learning for stochastic dynamical systems, National Science Foundation, Mathematical Sciences Graduate Internship, Summer 2022.

Sen Lin (University of Houston): Anomaly detection in dynamical systems using Bayesian online changepoint detection, Givens Associateship, Summer 2022.

Cyril Le Doux (University of Chicago): Deep learning emulators for geophysical modeling, DOE Summer Undergraduate Internship (SULI), Summer 2022.

Gurpreet Singh Hora (Columbia University): Adaptive training of deep learning surrogates in OpenFOAM (with Laurent White at AMD Research), Summer 2022.

Sahil Bhola (University of Michigan): Multifidelity reinforcement learning for computational fluid dynamics, Research Aide, Summer 2021.

Alec Linot (University of Wisconson): Deep learning of dynamical systems on inertial manifolds, Wallace Givens Associate, Summer 2021.

William McClure (IIT-Chicago): Estimating the Generator of SDEs Using Temporal Normalizing Flows, Masters Thesis, 2021.

Janah Richardson: Causal Relationship Between Environmental Factors and Social Mobility, Argonne mentor for the Afro-Academic, Cultural, Technological and Scientific Olympics (ACT-SO) High School Research Program, 2020-2021. Gold medal winner in Computer Science category- Illinois.

Suraj Pawar (Oklahoma State): Scalable reinforcement learning for computational fluid dynamics, Research Aide, 2020.

Dominic Skinner (MIT): Deep learning reduced-order models for computational physics applications, National Science Foundation, Mathematical Sciences Graduate Internship, Summer 2020.

# Publications

## *Under review*

1. C. Moss, R. Maulik, G. V. Iungo: Modeling Wind Turbine Performance and Wake Interactions with Machine Learning.
2. C. Moss, M. Puccioni, **R. Maulik**, C. Jacquet, D. Apgar, G. V. Iungo : Predicting Wind Farm Operations with Machine Learning and the P2D-RANS model: A Case Study for an AWAKEN Site,
3. S. Bhola, S. Pawar, P. Balaprakash, **R. Maulik**: Multi-fidelity reinforcement learning framework for shape optimization, *arXiv:2202.11170*.

4. S. Mondal, G. Magnotti, B. Lusch, **R. Maulik**, R. Torelli: A physics-consistent machine learning model with uncertainty propagation to predict spatiotemporal boundary conditions for coupled simulations.

5. A. Aygun, **R. Maulik**, A. Karakus: Physics-Informed Neural Networks for Mesh Deformation with Exact Boundary Enforcement, *arXiv:2301.05926*.

## *Peer-reviewed journal articles*

1. V. Shankar, V. Puri, R. Balakrishnan, **R. Maulik**, V. Vishwanathan: Differentiable physics-enabled closure modeling for Burgers' turbulence, *Machine Learning Science and Technology, Accepted*, 2023.

2. Politics of Problem Definition: Comparing Public Support of Climate Change Mitigation Policies using Machine Learning, J. Choi, W. Wehde, **R. Maulik**, *Review of Policy Research (Accepted)*, 2022.

3. S. Mondal, G. Magnotti, B. Lusch, **R. Maulik**, R. Torelli: Machine Learning-Enabled Prediction of Transient Injection Map in Automotive Injectors With Uncertainty Quantification, *Journal of Engineering for Gas Turbines and Power*, 145(4), 041015, 2023

4. A. Linot, J. Burby, Q. Tang, P. Balaprakash, M. Graham, **R. Maulik**: Stabilized Neural Ordinary Differential Equations for Long-Time Forecasting of Dynamical Systems, *Journal of Computational Physics*, 474, 111838, 2022.

5. N. Garland, **R. Maulik**, Q. Tang, X. Tang, P. Balaprakash, Efficient training of artificial neural network surrogates for a collisional-radiative model through adaptive parameter space sampling, *Machine Learning Science and Technology*, 3 (4), 045003, 2022.

6. M. Morimoto, K. Fukami, **R. Maulik**, R. Vinuesa, K. Fukagata: Assessments of model-form uncertainty using Gaussian stochastic weight averaging for fluid-flow regression, *Physica D: Nonlinear Phenomena*, 133454, 2022.

7. A. Lario, **R. Maulik**, G. Rozza, G. Mengaldo: Neural-network learning of SPOD dynamics, *Journal of Computational Physics*, 111475, 2022.

8. G. Iungo, **R. Maulik**, S. Renganathan, S. Letizia: Machine-learning identification of the variability of mean velocity and turbulence intensity for wakes generated by onshore wind turbines: Cluster analysis of wind LiDAR measurements, *Journal of Renewable and Sustainable Energy*, 14 (Cover article), 023307, 2022.

9. **R. Maulik**, V. Rao, J. Wang, G. Mengaldo, E. Constantinescu, B. Lusch, P. Balaprakash, I. Foster, R. Kotamarthi, Efficient high-dimensional variational data assimilation with machine-learned reduced-order models, *Geoscientific Model Development*, 15, 3433–3445, 2022..

10. Y. Lu, **R. Maulik**, T. Gao, F. Dietrich, I. Kevrekidis, J. Duan: Learning the temporal evolution of multivariate densities via normalizing flows, *Chaos: An Interdisciplinary Journal of Nonlinear Science*, 32 (3), 033121, 2022.

11. **R. Maulik**, D. Fytanidis, B. Lusch, S. Patel, V. Vishwanath: PythonFOAM: In-situ data analyses with OpenFOAM and Python, *Journal of Computational Science*, 62, 101750, 2022.

12. S. Renganathan, **R. Maulik**, G. Iungo, S. Letizia: Data-driven wind turbine wake modeling using probabilistic machine learning, *Neural Computing and Applications*, 34, 6171–618, 2022.

13. K. Lyras, **R. Maulik**, D. Schmidt: Machine-learning accelerated turbulence modelling of transient flashing jets, *Physics of Fluids*, 33, 127104 (2021).

14. K. Fukami, **R. Maulik**, N. Ramachandra, K. Taira, K. Fukagata: Global field reconstruction from sparse sensors with Voronoi tessellation-assisted deep learning, *Nature Machine Intelligence*, 2021.
15. B. Hamzi, **R. Maulik**, H. Owhadi: Simple, low-cost, and accurate, data-driven geophysical forecasting with learned kernels, *Proceedings of the Royal Society A*, 477: 20210326, 2021.
16. G. Mengaldo, **R. Maulik**, PySPOD: A Python package for Spectral Proper Orthogonal Decomposition (SPOD), *Journal of Open Source Software*, 6 (60), 2862, 2021.
17. **R. Maulik**, B. Lusch, P. Balaprakash: Reduced-order modeling of advection-dominated systems with recurrent neural networks and convolutional autoencoders , *Physics of Fluids*, 33, 037106, 2021 (Editor's pick).
18. S. Pawar, **R. Maulik**: Distributed deep reinforcement learning for simulation control, *Machine Learning: Science and Technology*, 2, 025029, 2021.
19. S. Renganathan, **R. Maulik**, J. Ahuja: Enhanced data efficiency using deep neural networks and Gaussian processes for aerodynamic design optimization, *Aerospace Science and Technology*, 111, 106522, 2021.
20. J. Burby, Q. Tang, **R. Maulik**: Fast neural Poincaré maps for toroidal magnetic fields, *Plasma Physics and Controlled Fusion*, 63, 024001, 2021.
21. **R. Maulik**, T. Botsas, N. Ramachandra, M. Lachlan, I. Pan: Latent-space time evolution of non-intrusive reduced-order models using Gaussian process emulation, *Physica D: Nonlinear Phenomena*, 132797, 2021.
22. **R. Maulik**, H. Sharma, S. Patel, B. Lusch, E. Jennings : A turbulent eddy-viscosity surrogate modeling framework for Reynolds-Averaged Navier-Stokes simulations, *Computers and Fluids*, 104777, 2020.
23. **R. Maulik**, K. Fukami, N. Ramachandra, K. Fukagata, K. Taira : Probabilistic neural networks for fluid flow surrogate modeling and data recovery, *Physical Review Fluids*, 5, 104401, 2020.
24. **R. Maulik**, P. Balaprakash, B. Lusch: Non-autoregressive time-series methods for stable parameteric reduced-order models, *Physics of Fluids*, 32, 087115, 2020 (Editor's pick).
25. **R. Maulik**, N. Garland, X. Tang, P. Balaprakash: Neural network representability of fully ionized plasma fluid model closures, *Physics of Plasmas*, 27, 072106, 2020.
26. J. Choi, S. Robinson, **R. Maulik**, W. Wehde: What Matters the Most for Individual Disaster Preparedness? Understanding Emergency Preparedness Using Machine Learning, *Natural Hazards*, 103, 1183-1200, 2020.
27. S. Renganathan **R. Maulik**, V. Rao : Machine learning for nonintrusive model order reduction of the parametric inviscid transonic flow past an airfoil, *Physics of Fluids*, 32, 047110, 2020.
28. **R. Maulik**, O. San: Numerical assessments of a parametric implicit large eddy simulation model, *Journal of Computational and Applied Mathematics*, 112866, 2020.
29. **R. Maulik**, O. San, J. Jacob: Spatiotemporally dynamic implicit large eddy simulation using machine learning classifiers, *Physica D: Nonlinear Phenomena*, 406, 132409, 2020.
30. **R. Maulik**, A. Mohan, B. Lusch, S. Madireddy, P. Balaprakash, D. Livescu: Time-series learning of latent-space dynamics for reduced-order model closure, *Physica D: Nonlinear Phenomena*, 405, 132368, 2020.

31. Y. Hossain, **R. Maulik**, H. Park, M. Ahmed, C. Bach, O. San: Improvement of Unitary Equipment and Heat Exchanger Testing Methods, *ASHRAE Transactions*, 125.2, 2019.
32. **R. Maulik**, O. San, J. Jacob, C. Crick: Sub-grid scale model classification and blending through deep learning, *Journal of Fluid Mechanics*, 870, 784-812, 2019.
33. O. San, **R. Maulik**, M. Ahmed: An artificial neural network framework for reduced order modeling of transient flows, *Communications in Nonlinear Science and Numerical Simulation*, 77, 271-287, 2019.
34. **R. Maulik**, O. San, A. Rasheed, P. Vedula: Subgrid modeling for two-dimensional turbulence using artificial neural networks, *Journal of Fluid Mechanics*, 858, 122-144, 2019.
35. **R. Maulik**, O. San, A. Rasheed, P. Vedula: Data-driven deconvolution for large eddy simulation of Kraichnan turbulence, *Physics of Fluids*, 30, 125109, 2018.
36. O. San, **R. Maulik**: Stratified Kelvin-Helmholtz turbulence of compressible shear flows, *Nonlinear Processes in Geophysics*, 25, 457–476, 2018.
37. O. San, **R. Maulik**: Extreme learning machine for reduced order modeling of turbulent geophysical flows, *Physical Review E*, 97, 042322, 2018.
38. O. San, **R. Maulik**: Machine learning closures for model order reduction of thermal fluids, *Applied Mathematical Modelling*, 60, 681-710, 2018.
39. **R. Maulik**, O. San, R. Behera : An adaptive multilevel wavelet framework for scale-selective WENO reconstruction schemes, *International Journal of Numerical Methods in Fluids*, 87 (5), 239-269, 2018.
40. O. San, **R. Maulik**: Neural network closure models for nonlinear model order reduction, *Advances in Computational Mathematics*, 44, 1717-1750, 2018.
41. **R. Maulik**, O. San: A dynamic closure modeling framework for large eddy simulation using approximate deconvolution: Burgers equation, *Cogent Physics*, 5, 1464368, 2018.
42. **R. Maulik**, O. San: A neural network approach for the blind deconvolution of turbulent flows, *Journal of Fluid Mechanics*, 831, 151-181, 2017.
43. **R. Maulik**, O. San: A novel dynamic framework for subgrid-scale parametrization of mesoscale eddies in quasigeostrophic turbulent flows, *Computers and Mathematics with Applications*, 74, 420-445, 2017.
44. **R. Maulik**, O. San: Explicit and implicit LES closures for Burgers turbulence, *Journal of Computational and Applied Mathematics*, 327, 12-40, 2017.
45. **R. Maulik**, O. San: Resolution and energy dissipation characteristics of implicit LES and explicit filtering models for compressible turbulence, *Fluids*, 2(2)-14, 2017.
46. **R. Maulik**, O. San: A dynamic subgrid-scale modeling framework for Boussinesq turbulence, *International Journal of Heat and Mass Transfer*, 108, 1656-1675, 2017.
47. **R. Maulik**, O. San: A dynamic framework for functional parameterisations of the eddy viscosity coefficient in two-dimensional turbulence, *International Journal of Computational Fluid Dynamics*, 31(2), 69-92, 2017.
48. **R. Maulik**, O. San: A stable and scale-aware dynamic modeling framework for subgrid-scale parameterizations of two-dimensional turbulence, *Computers & Fluids* 158, 11-38, 2016.
49. **R. Maulik**, O. San: Dynamic modeling of the horizontal eddy viscosity coefficient for quasigeostrophic ocean circulation problems, *Journal of Ocean Engineering and Science* 1, 300-324, 2016.

50. H. H. Marbini, **R. Maulik**: A biphasic transversely isotropic poroviscoelastic model for the unconfined compression of hydrated soft tissue, *Journal of Biomechanical Engineering* 138, 031003, 2016.

## *Peer-reviewed conference publications*

1. R. Egele, **R. Maulik**, K. Raghavan, P. Balaprakash, B. Lusch, AutoDEUQ: Automated Deep Ensemble with Uncertainty Quantification, *Accepted, International Conference on Pattern Recognition 2022, arXiv:2110.13511*.

2. Sudeepta Mondal, Gina M. Magnotti, Bethany Lusch, **Romit Maulik**, Roberto Torelli: Machine Learning-Enabled Prediction of Transient Injection Map in Automotive Injectors With Uncertainty Quantification, ASME Internal Combustion Engine Fall Conference, 2021.

3. H. Shan, Y. Sun, **R. Maulik**, T. Xu: Application of Artificial Neural Network in the APS LINAC Bunch Charge Transmission Efficiency, *12th International Particle Accelerator Conference (IPAC), 2021.*, `https://accelconf.web.cern.ch/ipac2021/papers/tupab287.pdf`.

4. V. Sastry, **R. Maulik**, V. Rao, B. Lusch, S. Renganathan, R. Kotamarthi: Data-driven deep learning emulators for geophysical forecasting, *International Conference on Computational Science, 433-446, 2021*, `https://doi.org/10.1007/978-3-030-77977-1_35`. Acceptance rate: 30.7%.

5. **R. Maulik**, R. Egele, B. Lusch, P. Balaprakash: Recurrent neural network architecture search for geophysical emulation, *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC), 2020, 10.5555/3433701.3433711*. Acceptance rate: 20%.

6. V. Rao, **R. Maulik**, E. Constantinescu, M. Anitescu: A machine learning method for computing rare event probabilities, *International Conference on Computational Science, 169-182, 2020*, `https://link.springer.com/chapter/10.1007%2F978-3-030-50433-5_14`. Acceptance rate: 30.7%.

7. **R. Maulik**, O. San, C. Bach: A computational investigation of the effect of ground clearance in vertical ducting systems, International High Performance Buildings Conference, Herrick Laboratories, Purdue University, 2018.
`https://docs.lib.purdue.edu/ihpbc/308/`.

## *Conference publications*

1. **R. Maulik**, H. Sharma, S. Patel, B. Lusch, E. Jennings: Deploying deep learning in OpenFOAM with TensorFlow: A tutorial, AIAA SciTech Forum 2021, `https://doi.org/10.2514/6.2021-1485`.

2. P. Milan, R. Torelli, B. Lusch, **R. Maulik**, G. Magnotti: Data-Driven Modeling of Large-Eddy Simulations for Fuel Injector Design, AIAA SciTech Forum 2021,
`https://doi.org/10.2514/6.2021-1016`.

3. **R. Maulik**, V. Rao, S. Renganathan, S. Letizia, G. Iungo: Cluster analysis of wind turbine wakes measured through a scanning Doppler wind LiDAR, AIAA SciTech Forum 2021,
`https://doi.org/10.2514/6.2021-1181`.

## *Peer-reviewed workshop proceedings*

1. **R. Maulik**, G. Mengaldo: PyParSVD: A streaming, distributed and randomized singular-value-decomposition library, (Accepted at 7th International Workshop on Data Analysis and Reduction for Big Scientific Data (DRBSD-7), Supercomputing 2021) *arXiv:2108.08845*.

2. D. Skinner, **R. Maulik**: Meta-modeling strategy for data-driven forecasting, *Tackling Climate Change with Machine Learning Workshop, NeurIPS*, 2020. `https://www.climatechange.ai/papers/neurips2020/13.html`.

3. N. Garland, **R. Maulik**, Q. Tang, X. Tang, P. Balaprakash: Progress towards high fidelity collisional-radiative model surrogates for rapid in-situ evaluation, *Machine Learning for Physical Sciences Workshop, NeurIPS*, 2020. `https://ml4physicalsciences.github.io/2020/files/NeurIPS_ML4PS_2020_79.pdf`.

4. K. Fukami, **R. Maulik**, N. Ramachandra, K. Fukagata, K. Taira: Probabilistic neural network-based reduced-order surrogate for fluid flows, *Machine Learning for Physical Sciences Workshop, NeurIPS*, 2020. `https://ml4physicalsciences.github.io/2020/files/NeurIPS_ML4PS_2020_7.pdf`

5. **R. Maulik**, R. S. Assary, P. Balaprakash: Site-specific graph neural network for predicting protonation energy of oxygenate molecules, *Machine Learning for Physical Sciences Workshop, NeurIPS*, 2019. `https://ml4physicalsciences.github.io/2019/files/NeurIPS_ML4PS_2019_134.pdf`

6. **R. Maulik**, V.Rao, S. Madireddy, B. Lusch, P. Balaprakash: Using recurrent neural networks for non-linear component computation in advection-dominated reduced-order models, *Machine Learning for Physical Sciences Workshop, NeurIPS*, 2019. `https://ml4physicalsciences.github.io/2019/files/NeurIPS_ML4PS_2019_99.pdf`.

## Talks presented

1. Accelerating scientific discovery using physics-informed machine learning, **Invited talk**, Machine Learning for e-Science, Swedish e-Science Research Centre, November 30, 2022.

2. Efficient high-dimensional variational data assimilation with machine-learned reduced-order models, Bulletin of the American Physical Society, Division of Fluid Dynamics, November, 2022.

3. A stabilized neural ordinary differential equation for scientific machine learning, **Invited talk**, SIAM Mathematics of Data Science, San Diego, September 28, 2022.

4. Neural forecasting of high-dimensional dynamical systems, **Invited talk**, University of Pittsburgh Computational Mathematics Seminar, September 20, 2022.

5. Quantifying Uncertainty in Deep Learning for Fluid Flow Reconstruction, **Invited talk**, USACM Thematic Conference on Uncertainty Quantification for Machine Learning Integrated Physics Modeling (MLIP), Crystal City, Virginia, August 18-19, 2022.

6. A stabilized neural ordinary differential equation for scientific machine learning, **Invited talk**, Argonne Training Program on Exascale Computing (ATPESC), August 12, 2022.

7. Learning nonlinear dynamical systems from data using scientific machine learning, **Invited talk**, 2022 AI + Science Summer School, University of Chicago, Data Sciences Institute, August 9, 2022.

8. Learning Nonlinear Dynamical Systems from Data Using Scientific Machine Learning, **Invited talk**, Accurate ROMs for Industrial Applications, Virginia Tech, July 7, 2022.

9. Non-intrusive reduced-order modeling using scientific machine learning, **Invited talk**, Summer School on Reduced Order Methods in CFD, SISSA Trieste, July 13, 2022.

10. Learning nonlinear dynamical systems from data using scientific machine learning, **Invited talk**, Brown University CRUNCH Seminar series, May 27, 2022.

11. Simple, low-cost and accurate data-driven geophysical forecasting with learned kernels, **Invited talk**, SIAM UQ, Atlanta, Georgia, April 12, 2022.
12. Reduced-order modeling of high-dimensional dynamical systems using scientific machine learning, **Invited talk**, IBiM Seminar Series, March 2022.
13. Emulating nonlinear dynamical systems from data using scientific machine learning, **Invited talk**, APS March Meetings, March 14, 2022.
14. Reduced-order modeling of high-dimensional dynamical systems using scientific machine learning, **Invited talk**, National University of Singapore, Department of Mechanical Engineering, Distinguished Seminar Series, February 10, 2022.
15. Emulating complex systems from data using scientific machine learning, **Invited talk**, North Carolina State University, Department of Mathematics, February 1, 2022.
16. Research at the intersection of mathematics, computation, and data, **Invited webinar**, BIT Mesra Alumni Association North America Faculty Webinar, January 29, 2022.
17. Reduced-order modeling of high-dimensional systems using scientific machine learning, **Invited talk**, IIT-Chicago MMAE Seminar Series, January 27, 2022.
18. Reduced-order modeling of high-dimensional systems using scientific machine learning, **Invited talk**, University of Waterloo, Department of Applied Mathematics, January 18, 2022.
19. Reduced-order modeling of high-dimensional systems using scientific machine learning, **Invited talk**, Florida State university, Department of Scientific Computing, November 19, 2021.
20. Research at the intersection of mathematics, computation, and data, **Invited talk**, Physics & Engineering speaker series, North Park University, November 17, 2021.
21. Reduced-order modeling of high-dimensional systems using machine learning, **Invited talk**, Civil and Environmental Engineering Seminar Series, Duke University, November 12, 2021.
22. Reduced-order modeling of high-dimensional systems using scientific machine learning, **Invited talk**, 2021 CBE Computing Seminar Series, University of Wisconsin-Madison, October 22, 2021.
23. Parallelized emulator discovery and uncertainty quantification using DeepHyper, Mechanistic Machine Learning and Digital Twins for Computational Science, Engineering & Technology, September 26-29, 2021.
24. Modified neural ordinary differential equations for stable learning of chaotic dynamics, **Invited talk**, Applied Mathematics Seminar Series, Texas Tech University, September 1, 2021.
25. Neural architecture search for surrogate modeling, **Invited talk**, ML4I Forum, Lawrence Livermore National Laboratory, August 10-12, 2021.
26. Scalable scientific machine learning for computational fluid dynamics, **Plenary talk**, Computational Sciences and AI in Industry, June 7-9, 2021.
27. Neural architecture search for surrogate modeling, **Invited talk**, DDPS Seminar Series, Lawrence Livermore National Laboratory, May 27, 2021.
28. Incorporating inductive biases for the surrogate modeling of dynamical systems, **Invited talk** at Machine Learning for Dynamical Systems Special Interest Group, Alan Turing Institute, Imperial College London, April 14, 2021.

29. Surrogate modeling with learned kernels (Kernel Flows), **Invited talk**, Uncertainty Quantification in Climate Science, NASA JPL Climate Center Virtual Workshop, March 24, 2021.
30. Scalable recurrent neural architecture search for geophysical emulation, **Invited talk** at SIAM-CSE Minisymposium on Physics-Guided Machine Learning and Data-Driven Methods in Computational Geoscience.
31. Incorporating Inductive Biases as Hard Constraints for Scientific Machine Learning, MCS-LANS seminar, Argonne National Laboratory, February 2021.
32. Scalable scientific machine learning for computational fluid dynamics, **Invited talk**, Department of Mechanical Engineering, The City College of New York, October, 2020.
33. Data-driven model order reduction for geophysical emulation. **Invited talk** at the Second Symposium on Machine Learning and Dynamical Systems, Fields Institute, Toronto, September, 2020.
34. Scalable scientific machine learning for computational fluid dynamics, **Invited talk**, Department of Mechanical Engineering, Rice University, September, 2020.
35. Machine Learning Enablers for System Optimization and Design, MCS-LANS seminar, Argonne National Laboratory, August 2020.
36. Surrogate-based machine-learning for system optimization and design, **Invited talk** at Los Alamos National Laboratory for Tokamak Disruption Simulation (TDS) working group, August, 2020.
37. Non-intrusive reduced-order model search for geophysical emulation, **Guest lecture**, MAE259a: Data science for fluid dynamics (offered by Kunihiko Taira), University of California Los Angeles, June 2020.
38. Spatiotemporally dynamic implicit large eddy simulation using machine learning classifiers, Session on Domain-Aware, Interpretable and Robust Scientific Machine Learning Methods Applied to Computational Mechanics, AIAA Aviation Forum, June, 2020, Reno.
39. Machine learning for computational fluid dynamics, **Invited talk** at PyData Meetup Chicago, May 2020.
40. Recurrent neural architecture search for geophysical emulation using DeepHyper, **Invited talk** at AI-HPC seminar, Argonne National Laboratory, April, 2020.
41. Machine Learned Reduced-Order Models for Advective Partial Differential Equations, MCS-LANS seminar, Argonne National Laboratory, February, 2020.
42. Machine Learned Reduced-Order Models for Advective Partial Differential Equations, **Invited talk**, 2020 Spring Multiscale Seminar, Illinois Institute of Technology, Chicago, February, 2020.
43. General purpose data science for general purpose CFD: Integrating Tensorflow into OpenFOAM at scale, **Invited poster**, Workshop for Machine Learning for Transport Phenomena, February, 2020, Dallas.
44. Machine learning of sequential data for non-intrusive reduced-order models, Bulletin of the American Physical Society, Division of Fluid Dynamics, November, 2019.
45. Tackling the limitations of conventional ROMs for advection-dominated nonlinear dynamical systems using machine learning, **Invited talk**, Advanced Statistics meets Machine Learning-III workshop, Argonne National Laboratory, November, 2019.

46. Data-driven sub-grid models for the large-eddy simulation of turbulence, **Invited talk**, John Zink Hamworthy Combustion, Tulsa, August, 2019.
47. Novel turbulence closures using physics-informed machine learning, Argonne Physical Sciences and Engineering Division AI Townhall, July, 2019.
48. Data-driven deconvolution for the sub-grid modeling of large eddy simulations of two-dimensional turbulence, SIAM-CSE, March, 2019.
49. Data-driven deconvolution for the large eddy simulation of Kraichnan turbulence, Bulletin of the American Physical Society, Division of Fluid Dynamics, November, 2018.
50. A computational investigation of the effect of ground clearance in vertical ducting systems, 2018, Purdue University, Herrick Labs Conferences, July, 2018.
51. A neural network approach for the blind deconvolution of turbulent flows, Bulletin of the American Physical Society, Division of Fluid Dynamics, November, 2017.
52. A generalized wavelet based grid-adaptive and scale-selective implementation of WENO schemes for conservation laws, Texas Applied Mathematics and Engineering Symposium, The University of Texas, Austin, September 2017.
53. An explicit filtering framework based on Perona-Malik anisotropic diffusion for shock capturing and subgrid scale modeling of Burgers' turbulence, Bulletin of the American Physical Society, Division of Fluid Dynamics, November, 2016.
54. A dynamic hybrid subgrid-scale modeling framework for large eddy simulations, Bulletin of the American Physical Society, Division of Fluid Dynamics, November, 2016.

# Professional service

## *Committee membership*

PythonFOAM Workshop Lead Organizer (https://www.alcf.anl.gov/events/alcf-pythonfoam-workshop).

DOE INCITE program (2020) - Reviewed 2 proposals every year

ADSP program (2020) - Reviewed 2 proposals every year

International Conference on Parallel Processing, Chicago, 2021 (Reviewed 6 articles).

Wilkinson Postdoctoral Fellowship Committee, MCS Division, Argonne National Laboratory, 2022.

DOE AI for Earth System Predictability workshop session chair for neural networks.

## *Tutorials organized*

Tutorial lead - Autoencoders for PDE surrogate models, ATPESC 2020.

Tutorial lead - Statistical methods for machine learning, ALCF AI4Science tutorial 2019, Argonne National Laboratory.

Tutorial lead - DeepHyper for scalable hyperparameter and neural architecture search on ALCF machines, ALCF Simulation Data and Learning workshop 2019, Argonne National Laboratory.

TensorFlow workshop, Mechanical & Aerospace Engineering, Oklahoma State University, 2018.

An introduction to high performance computing for middle school kids, National Lab Day, Oklahoma State University 2017, 2018.

### *Minisymposia*

Organizer - Acceleration and Enhancement of High-fidelity PDE Solvers through Machine Learning, 16th U.S. National Congress on Computational Mechanics, IL, 2021.

Co-organizer - Argonne National Laboratory - AI, Statistics and Machine Learning Journal Club.

Session chair - Domain-Aware, Interpretable and Robust Scientific Machine Learning Methods Applied to Computational Mechanics, AIAA Aviation Forum, Reno, NV, 2020.

MS Organizer & Session chair - Domain-Aware, Interpretable and Robust Machine Learning for Computational Science, SIAM-CSE, 2021.

MS Organizer & Session chair - Machine Learning methods in Computational Fluid Dynamics, SIAM-CSE, Spokane, WA, 2019.

Session chair - MAE Graduate Research Symposium, Oklahoma State University, 2018.

### *Journal Review*

Journal reviewer for - AIAA Journal, Applied Mathematical Modeling, Chaos, Computer Methods in Applied Mathematics and Engineering, Communications in Computational Physics, Computers and Fluids, Computer Physics Communications, International Journal of Computational Fluid Dynamics, IEEE Transactions on Plasma Science, Journal of Fluid Mechanics, Journal of Scientific Computing, Physics of Fluids, Physica D, International Journal of Numerical Methods in Fluids, Journal of Computational Physics, Journal of Nonlinear Science, Nature Communications, Nature Machine Intelligence, Nature Scientific Reports, Theoretical and Computational Fluid Dynamics, Atmospheric Science Letters, New Journal of Physics.

## Software developed

1. R. Maulik, D. Fytanidis, S. Patel, B. Lusch, V. Vishwanath, PythonFoam: In-situ data analyses with OpenFOAM and Python. `https://github.com/argonne-lcf/PythonFOAM`.

2. R. Maulik, H. Sharma, S. Patel, B. Lusch, E. Jennings, TensorFlowFoam: A framework that enables the deployment of deep learning (in Python) and partial differential equation solutions concurrently in OpenFOAM - a C++-based open-source finite-volume based computational physics package. `https://github.com/argonne-lcf/TensorFlowFoam`.

3. R. Maulik, S. Pawar, PAR-RL: A framework that leverages the Ray library to deploy scalable deep reinforcement learning for arbitrary scientific environments on leadership class machines. Tested on ALCF supercomputer Theta for controlling simulations of dynamical systems. `https://github.com/Romit-Maulik/PAR-RL`.

4. R. Maulik, G. Mengaldo, PyParSVD: A Parallelized, streaming, and randomized implementation of the SVD for Python using mpi4py. `https://github.com/Romit-Maulik/PyParSVD`. DOI: 10.5281/zenodo.4562889.

5. G. Mengaldo, R. Maulik, PySPOD: Python Spectral Proper Orthogonal Decomposition. `https://github.com/mengaldo/PySPOD`. DOI: https://doi.org/10.21105/joss.02862.